

Interacting electrons in a magnetic field in a center-of-mass free basis.

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Abstract

We present an extension of the spin-adapted configuration-interaction method for the computation of four electrons in a quasi two-dimensional quantum dot. By a group-theoretical decomposition of the basis set and working with relative and center-of-mass coordinates we obtain an analytical identification of all spurious center-of-mass states of the Coulomb-interacting electrons. We find a substantial reduction in the basis set used for numerical computations. At the same time we increase the accuracy compared to the standard spin-adapted configuration-interaction method (SACI) due to the absence of distortions caused by an unbalanced cut-off of center-of-mass excitations.

Dedicated to Margarita and Vladimir Man'ko on the occasion of their 150th birthday.

1 Introduction.

The Schrödinger equation of an interacting many-body system can be solved analytically only for specific interaction potentials and for a very restricted number of particles. A wide range of approximation methods has been developed to determine the ground and excited states of many-body systems found in nuclear, atomic, and condensed matter systems. Here, we focus on quasi two-dimensional electronic systems, which are experimentally realized in quantum-dots. Quantum dots are often embedded in layered semiconductor structures. The strong confinement along the vertical direction perpendicular to the layer suggests an effectively two-dimensional description along the remaining two lateral dimensions. Besides the electron-electron interactions, an additional external confinement potential along the lateral directions

is created by etching and gating of the semiconductor device. Quantum dots can be regarded as *artificial atoms*, albeit with a central potential different from the nuclear Coulomb attraction. Their excitation spectra are probed by electronic and optical measurements, also under the influence of additional magnetic fields, which gives rise to a Landau-level structure.

With the discovery of the fractional Quantum Hall effect (FQHE) in systems of interacting electrons in quasi two-dimensional systems, many theoretical approaches for studying interacting electrons have been proposed, including the celebrated Laughlin wave-function for electrons in the lowest Landau level. In the experimentally realized Hall devices translational symmetry is broken by the current source and drain contacts, which lead to the formation of hot-spots with high electric field values [21, 22].

A comparison of the various theoretical approaches with numerical methods is often performed for few-electron quantum dots. Analytic [33, 30] and numerical [34] solutions for the two electron case show the interplay of Coulomb interaction and confinement potential, leading to alternating spin polarization of the ground state in a quantum-dot as function of magnetic field [29]. By separation of the two-electron case into the center-of-mass motion and the relative part, semiclassical solutions have been constructed [12] and compared to the exact solutions [20, 8, 7]. For three electrons, the relative-coordinate basis set and expressions for the Coulomb matrix elements are given in [32].

In the popular *configuration interaction* (CI) approach a diagonalization of the Hamiltonian including the Coulomb-interaction is done with respect to a product basis of single-particle Slater determinants. Convergence is generally checked by systematically enlarging the size of the basis set, for instance by increasing the value of the cut-off energy up to which all states are included for the non-interacting system [31]. With increasing number of basis states, the computation of all interacting matrix-elements and the final diagonalization of the Hamiltonian quickly exhausts computer resources. Thus a reduction of the basis set while maintaining accuracy is required for studying the excitation spectra of few body systems.

If the reduction is based on underlying group-theoretical properties, an exact decomposition of the basis set into irreducible blocks is possible. A diagonalization of the smaller blocks is more easily achievable and the decomposition provides physical insight into the system.

One example is the separation of the spatial part of the wavefunction from the spinor states for electrons. If we require that the product of spatial and spin-part represents electrons (antisymmetric states), the basis set is decomposed into separate spin states. This results in spin-adapted (SA) configuration methods, for instance implemented in the SACI program code [27, 28].

At this point SACI methods used in condensed matter theory for more than 3 electrons stop and do not exploit additional properties of the basis set, such as a de-

composition into relative and (interaction-free) center-of-mass (cm) states. The separation of the basis set into a product state of relative and center-of-mass part is of particular use if the Hamiltonian of the n -electron system is given as a sum of operators acting on center-of-mass and relative coordinates respectively. For electrons confined to a two-dimensional plane perpendicular to a uniform magnetic field this separation of the Hamiltonian is possible as long as the confinement potential in the two-dimensional plane does not lead to an admixing of relative and center-of-mass coordinates [13, 2]. For molecular or atomic systems moving in three dimensions across uniform magnetic fields, additional couplings between relative and center-of-mass coordinates occur, i.e. the motional Stark effect [11, 38, 7]. The importance of a systematic separation of relative coordinates from the center-of-mass excitation for studying correlated two-dimensional electron systems for three electrons was pointed out early by Laughlin [24] and noticed recently again for more than three electrons [37]. Laughlin's trial wave function by construction is expressed only in relative coordinates and can be interpreted and numerically handled similar to a classical plasma of interacting particles [23].

We note that both in many-electron and nuclear physics, the interactions between the particles are exclusively functions of relative coordinates. Then the same shift vector applied to any single particle coordinate does not change the hamiltonian. By the well-known Noether theory of symmetry it then follows that the total momentum \mathbf{P} of the system is conserved. For an unusual but powerful example of a conserved quantity we refer to [19]. Relative coordinates, in contrast to the single particle coordinates, are free of the cm coordinate. In quantum mechanics, the components of \mathbf{P} are proportional to the partial derivatives of the cm coordinate. Therefore, if the states depend on relative coordinates only, we have $\mathbf{P} = \mathbf{0}$. Another possible option which we shall adopt is to demand the cm state to have zero oscillator excitation. The paradigms of nuclear theory show [14, 17, 1] that relative coordinates are the natural tools to understand and compute nuclear scattering and reactions. In nuclear structure, such coordinates may be adapted and serve to describe few-particle systems [16, 1], clustering, and decay processes. The construction of orbital states can be achieved by use of group and representation theory [17, 18]. The orbital states are coupled with spin states to antisymmetric states. The adaption to orbital permutational symmetry for composite systems in relative coordinates becomes more involved, but was extensively studied in [15].

We report here work on 2D electrons in an external perpendicular magnetic field, so that the 2D total momentum is still conserved [13, 2]. We use harmonic oscillator states and the methods of Bargmann Hilbert space. The electron-electron Coulomb repulsion is computed in matrix form and included into the diagonalization. For $n = 4$ electrons we use the relative tetrahedral coordinates from [14] with simple properties under permutations. The spin states for total spin $S = 2, 1, 0$ are explicitly determined by projection operators.

Single-particle coordinates are used to construct antisymmetric states as Slater determinants of single-particle states. If these states are taken as harmonic oscillator states, Slater determinants cannot avoid the intrusion of cm excitations into state space which give rise, in addition to the proper states, to so-called spurious states of spurious angular momentum. The true role of spurious states can be seen only by the parallel use of relative and cm coordinates. We shall present in section 7 in particular for total spin $S = 0$, a complete analysis of these spurious states. Their intrusion of state space is demonstrated in the spectrum of determinantal eigenstates of the standard SACI approach [27, 28, 31]. Moreover, if determinantal eigenstates are variationally computed in a subspace defined by a fixed maximal oscillator excitation, we find that the admixture of spurious states distorts this subspace and the variational results. In our proper treatment, any eigenstate in relative coordinates is the basis to a set of equidistant spurious states of increasing cm excitation.

2 Total spin S and orbital partition f .

The total spin of n electrons ranges from the maximum $S = n/2$ to the minimum value, $S = 1/2$ for n odd and $S = 0$ for n even. The permutational symmetry of the spin state is characterized by a partition $f^S = [f_1^S f_2^S]$, $f_1^S + f_2^S = n$, $f_1^S \geq f_2^S$ of two rows $[f_1^S, f_2^S]$ only, because there are for any electron only the two spin (up, down) states. The total spin S is related one-to-one to the spin partition f^S by

$$S(f^S) = \frac{1}{2}(f_1^S - f_2^S). \quad (1)$$

Since the electrons are fermions, the combined orbital plus spin state must be antisymmetric with partition $f = [11..1]$. Then it follows that the only allowed orbital partition f is associate to the spin partition f^S , that is, its Young diagram consists of n square boxes, arranged in f_2^S rows of length 2, and $(f_1^S - f_2^S)$ rows of length 1. To the orbital partition f there belong orthogonal partner functions whose number we denote by $|f|$. They may be labelled by Young tableaux r, s, \dots . Any Young tableau is a filling of the boxes of the Young diagram f by the numbers $1, 2, \dots, n$, such that the numbers increase both to the right and downwards. The application of permutations to an orbital state of n particles, denoted as $|\alpha^n f r\rangle$, is completely determined by the tableau r . The antisymmetric fermion state, with respect to permutations, takes the form of a sum of products of orbital and spin states,

$$|[1^n]\alpha^n S\rangle = |f|^{-\frac{1}{2}} \sum_r |\alpha^n f r\rangle |S f^S r^S\rangle, \quad (2)$$

where r^S is the Young tableau of the spin partition f^S , determined from the orbital tableau r by reflection in the main diagonal of its orbital Young diagram.

The operators O for the external magnetic field, the central field and the interactions are all invariant under permutations and independent of the spin. Since the spin basis states $|Sf^S r^S\rangle$ are orthogonal, the matrix elements of all spin-independent operators O between antisymmetric states reduce to the spin-free sum of orbital matrix elements

$$\langle 1^n S | O | 1^n S \rangle = |f|^{-1} \sum_r \langle \alpha^n f r | O | \alpha^n f r \rangle. \quad (3)$$

Here the total spin S is fixed from eq. 1 by half the difference of the column length of the orbital partition f . From eq. 3 it follows that we never need the spin states but must compute $|f|$ orbital diagonal matrix elements.

Example: For $n = 4$ particles, the possible values of the total spin are $S = 2, 1, 0$. The corresponding spin partitions are $f^S = [4], [31], [22]$, and the orbital partitions are $f = [1^4], [211], [22]$ of dimensions $|f| = 1, 3, 2$ respectively.

So we need the construction of $|f|$ orbital states with an orbital partition f , fixed by the total spin S , and by its Young tableaux r .

2.1 Orbital Young diagrams and representation of transpositions.

To project states of orbital symmetry f with the Young tableau r, s , we use the matrix elements of the representation $D_{r,s}^f(p)$ which are determined by the tableaux. A Young diagram is an arrangement of square boxes in rows of length $f_1 f_2 \dots f_n$. In a Young tableau r , we label these boxes by $1, 2, \dots, n$ such that the numbers increase to the right and downwards. There are exactly $|f|$ Young diagrams for the partition f . The row and column of the box i are then (α_i, β_i) . For a pair of boxes (i, j) we define the axial distance [15] p.28 by

$$\tau_{ij} = (\alpha_i - \alpha_j) - (\beta_i - \beta_j). \quad (4)$$

We first determine the matrices of the representation for the $(n-1)$ transpositions $p = (1, 2), (2, 3), \dots, (n-1, n)$ of $S(n)$. These transposition by multiplication generate all elements of $S(n)$, and so all representation matrices can be built by matrix multiplication from the representations of these transpositions. For the permutation which interchanges i with $j = i+1$ and the Young tableau r , there may be a second tableau s with boxes (i, j) interchanged. If there is no such second tableau, the two boxes must appear in succession in the same row or the same column of the Young tableau. In these two cases the matrix element of the representation are given by

$$D_{rs}^f(i, i+1) = 1/\tau_{i,i+1} = \pm 1. \quad (5)$$

Otherwise, the non-trivial part of the representation is given by the 2×2 matrix

$$d_{r,s}^f(i, i+1) = \begin{bmatrix} 1/\tau_{i,i+1} & \sqrt{1 - (\tau_{i,i+1})^{-2}} \\ \sqrt{1 - (\tau_{i,i+1})^{-2}} & -1/\tau_{i,i+1} \end{bmatrix}. \quad (6)$$

The operator of the transposition $T(p) = T(a, b)$ interchanges the coordinates of the single particle indexed by the number a with those of the particle indexed by b . Following the Wigner [36] pp.102-6 prescription, to assure a homomorphic action we must associate to any permutation p the inverse action $T(p)$ of the permutation on the particle indices.

The Young operators [15] pp. 25-26 are given by

$$c_{rs}^f = \frac{|f|}{n!} \sum_{p \in S(n)} D_{r,s}^f(p) T(p), [c_{rs}^f]^\dagger = c_{sr}^f. \quad (7)$$

These operators must be applied to the highest polynomials eq. 23 of fixed pseudo angular momentum Λ (see Sect. 3.2), provided that from [14] we know that Λ can yield the orbital partition f . If a Young operator gives zero when applied to the polynomial, we first apply a lowering operator eq. 25 and then again try the Young operator. Exhausting all values of the pseudo angular component we must find all the states of orbital symmetry.

For an antisymmetric state eq. 2 we use orbital transposition operators $T(s, t)$ to write

$$\sum_{s < t} V(s, t) = \sum_{s < t} T(s, 1) T(t, 2) V(1, 2) T(t, 2) T(s, 1), \quad (8)$$

$$\langle \alpha^n [1^n] S | \sum_{s < t} V(s, t) | \alpha^n [1^n] S \rangle \quad (9)$$

$$\begin{aligned} &= \frac{1}{|f|} \sum_{s < t} \sum_r \langle fr | T(s, 1) T(t, 2) V(1, 2) T(t, 2) T(s, 1) | fr \rangle \\ &= \frac{1}{|f|} \sum_{s < t} \sum_r \sum_{r', r''} \langle fr | T(s, 1) T(t, 2) | fr' \rangle \langle fr' | V(1, 2) | fr'' \rangle \langle fr'' | T(t, 2) T(s, 1) | fr \rangle \\ &= \frac{n(n-1)}{2} \frac{1}{|f|} \sum_r \langle fr | V(1, 2) | fr \rangle. \end{aligned}$$

The third line of eq. 8 follows from the orthogonality of the spin states in eq. 2. In the last line we use the involutive property of transpositions and the orthogonality of Young tableaux,

$$\begin{aligned} [T(s, 1)]^2 &= [T(t, 2)]^2 = 1, \\ \langle fr'' | fr' \rangle &= \delta_{r'', r'}. \end{aligned} \quad (10)$$

Prop: The matrix element of orbital twobody interactions, invariant under permutations, between antisymmetric states of fixed total spin S , can be reduced to a sum over diagonal orbital matrix elements of the interaction of the first pair between states characterized by Young tableaux, multiplied by the number of pairs.

To construct states with other tableaux of the same partition, we provide a ladder procedure by employing the properties of the representation. Given an initial basis function $|fr\rangle$, we know from eq. 6 that the permutation $(i, i+1)$ connects it at most to a second basis function $|fs\rangle$ whose Young tableau differs by an interchange of the numbers $(i, i+1)$. We rewrite eq. 6 in the form

$$\begin{aligned} T(i, i+1)|fr\rangle &= |fr\rangle\tau^{-1} + |fs\rangle\sqrt{1 - (\tau)^{-2}}, \\ |fs\rangle &= |fr\rangle\frac{-\tau^{-1}}{\sqrt{1 - (\tau)^{-2}}} + T(i, i+1)|fr\rangle\frac{1}{\sqrt{1 - (\tau)^{-2}}}. \end{aligned} \quad (11)$$

Therefore once we know how to apply $T(i, i+1)$ to the state $|fr\rangle$, we can construct $|fs\rangle$ as the linear combination eq. 11, second line. With the operator eq. 7 we have constructed the state with the highest Young tableau.

Prop: With steps as in eq. 11 we can generate all other Young tableaux from an initial one.

Examples are given in the following subsections.

2.2 Construction of permutations.

In an orbital Young operator eq. 7, the sum runs over all permutations of $S(n)$. This sum may be broken into classes k , characterized by i_1, i_2, \dots, i_n independent and commuting cyclic permutations of length 1, 2, ..., n where

$$1i_1 + 2i_2 + \dots + ni_n = n. \quad (12)$$

Any cyclic permutations in turn can be factorized into transpositions as

$$(abcd\dots) = (ab)(bc)(cd)(\dots) \quad (13)$$

and any transposition is conjugate to one of the n generators (12), (23), ... of $S(n)$, see eq. 30. By the representation $p \rightarrow D(p)$, all the factorizations of permutations are converted into matrix factorizations. A systematic enumeration of all $n!$ permutations can go in terms of classes k of conjugate elements. The number of permutations in the class k corresponding to eq. 12 according to Weyl [35] p.329 is

$$n(k) = \frac{n!}{1^{i_1}i_1!2^{i_2}i_2!\dots}. \quad (14)$$

3 Orbital states, unitary quantum numbers, total angular momentum.

For a single electron in 2D, we label its state by the oscillator excitation ν , by the numbers $n^+, n^-, n^+ + n^- = \nu$ of right and left circular oscillator quanta, and by the angular momentum $l = n^+ - n^-$.

Note the following relations for coordinates and derivatives of a single particle in 2D, passed to a circular setting:

$$\begin{aligned}
z^+ &:= \sqrt{\frac{1}{2}}(z^1 + iz^2), \quad z^- := \sqrt{\frac{1}{2}}(z^1 - iz^2), \\
z^1 &= \sqrt{\frac{1}{2}}(z^+ + z^-), \quad z^2 = -i\sqrt{\frac{1}{2}}(z^+ - z^-), \\
\partial^+ &= \sqrt{\frac{1}{2}}(\partial^1 - i\partial^2), \quad \partial^- = \sqrt{\frac{1}{2}}(\partial^1 + i\partial^2), \\
\partial^1 &= \sqrt{\frac{1}{2}}(\partial^+ + \partial^-), \quad \partial^2 = i\sqrt{\frac{1}{2}}(\partial^+ - \partial^-),
\end{aligned} \tag{15}$$

and the quadratic relations

$$\begin{aligned}
z^1\partial^1 + z^2\partial^2 &= z^+\partial^+ + z^-\partial^- \\
z^1z^1 + z^2z^2 &= z^+z^- + z^-z^+.
\end{aligned} \tag{16}$$

The last relations are easily extended to scalar products of several vectors, labelled and contracted wrt lower indices. These yield generators of the symplectic group $Sp(2, R)$.

The states of n electrons are then labelled by the summed up number N of oscillator quanta and by the summed up angular momentum

$$L = \sum_{s=1}^n (n_s^+ - n_s^-). \tag{17}$$

It is desirable to find other (integer) orbital quantum numbers which if possible can label at least in part an orthogonal set of orbital states. For this purpose we use the scheme of [14] whose quantum numbers arise from group representations. The unitary group of all orbital degrees of freedom is the unitary group $U(2n)$, its commuting subgroups acting on the 2 orbital or the $(n-1)$ relative motion degrees of freedom are $U(2) \times U(3)$. Their representations are both given by the same two-component integer partitions $[h_1 h_2]$, $h_1 + h_2 = N$, $h_1 \geq h_2 \geq 0$. The representation of the subgroup $SO(2) < U(2)$ is characterized by the angular momentum L . For given partition $[h_1 h_2]$ the angular momentum ranges from its maximum $L = h_1 - h_2$ to its minimum value 1 or 0 for $(h_1 - h_2)$ odd or even respectively.

3.1 Lowest Landau level LLL .

In the 2D magnetic field, the lowest Landau level LLL arises if the summed up angular momentum L equals the summed up excitation N . In terms of the partition

$[h_1 h_2]$ for the unitary group $U(2)$, we have $N = h_1 + h_2$. The weights, i.e. the degrees (w_1, w_2) of the vectors indexed 1, 2, are restricted to the range $h_1 \leq w_i \leq h_2$, and the maximum angular momentum is $L = \max(w_1 - w_2) = h_1 - h_2$. The lowest Landau level therefore enforces $h_1 - h_2 = h_1 + h_2, h_2 = 0$. This condition selects among the partitions of N the single case $[h_1 h_2] = [N 0], L = N$. Only for this partition can the excitation N be carried by a single vector. For higher Landau levels this condition is relaxed and new unitary partitions are allowed.

3.2 Pseudo angular momentum and lowering operators.

The group $U(3)$ has an orthogonal subgroup $SO(3)$ whose representation label we term the pseudo angular momentum Λ . The possible values of Λ were given in [4]. Here the authors use the subgroup chain

$$U(3) > SU(3) > SO(3), \quad (18)$$

with branching of representation labels

$$[h_1 h_2] > (\lambda', \mu') > \Lambda, \quad (\lambda', \mu') = (h_1 - h_2, h_2). \quad (19)$$

The range of these labels is determined by specific branchings from the representation in the next higher subgroup which we shall discuss in more detail.

We treat the oscillator states by the methods of Bargmann Hilbert space of analytic functions [15]. We specifically note that in what follows we must *interchange the role of the groups and subgroups* $U(2), U(3)$ compared to [4], and *convert angular into pseudo angular momentum*. This allows us to take advantage of the group theory given in [4], but in a new and different interpretation.

By *upper indices* $j = 1, 2$ (or upper \pm), see below, we denote the Cartesian vector components in 2D, and by *lower Cartesian indices* $s = (1, 2, 3)$ or spherical indices $(+, -, 0)$ three (or more) relative vectors of the four (or more) particles. The normalized states of angular momentum LM of a single particle with oscillator excitation N in the Bargmann representation are

$$P_{LM}^N(z) = A_{NL}(z \cdot z)^{\frac{1}{2}(N-L)} Y_{LM}(z), \quad A_{NL} = (-1)^{\frac{1}{2}(N-L)} \left[\frac{4\pi}{(N+L+1)!!(N-L)!!} \right]^{\frac{1}{2}}. \quad (20)$$

with $Y_{LM}(z)$ a solid spherical harmonic [6] p.69. The coordinates may then be taken as the six linear combinations of Cartesian coordinates

$$\begin{aligned} z_+^+ &= \sqrt{\frac{1}{2}} [(z_1^1 + iz_2^1) + i(z_1^2 + iz_2^2)], \\ z_-^+ &= \sqrt{\frac{1}{2}} [(z_1^1 - iz_2^1) + i(z_1^2 - iz_2^2)], \quad z_0^+ = z_3^+, \end{aligned} \quad (21)$$

$$z_+^- = \sqrt{\frac{1}{2}}[(z_1^1 + iz_2^1) - i(z_1^2 + iz_2^2)],$$

$$z_-^- = \sqrt{\frac{1}{2}}[(z_1^1 - iz_2^1) - i(z_1^2 - iz_2^2)], \quad z_0^- = z_3^-.$$

The lower Cartesian indices (1, 2, 3) denote three relative coordinates like the Jacobi or tetrahedral ones. The permutations of particles act on these coordinates and introduce linear combinations wrt the lower indices.

Next we introduce from [4] p.187 for $n = 4$ the elementary polynomials

$$\begin{aligned} \eta_+ &:= z_1^1 + iz_2^1, \\ v_+ &:= i(z_0^1 z_+^2 - z_0^2 z_+^1), \\ w_+ &:= [(z^1 \times z^2) \times z^1]_+ \\ s &:= z_+^1 z_-^1 + z_0^1 z_0^1, \\ t &:= (z^1 \cdot z^1)(z^2 \cdot z^2) - (z^1 \cdot z^2)^2, \end{aligned} \tag{22}$$

In [4] p. 187 we find in the scheme eq. 18 the linearly independent polynomials

$$\begin{aligned} &h_1 - \Lambda \text{ even :} \\ P_{h_1 h_2 \Lambda} &= \eta_+^{(\Lambda - h_2 + 2q)} v_+^{(h_2 - 2q)} s^{((h_1 - \Lambda)/2 - q)} t^q, \\ &0 \leq 2q \leq h_2, \\ &h_2 - \Lambda \leq 2q \leq h_1 - \Lambda \\ &h_1 - \Lambda \text{ odd :} \\ P_{h_1 h_2 \Lambda} &= w_+ \eta_+^{(\Lambda - h_2 + 2q)} v_+^{(h_2 - 1 - 2q)} s^{((h_1 - \Lambda - 1)/2 - q)} t^q, \\ &0 \leq 2q \leq h_2 - 1, \\ &h_2 - \Lambda \leq 2q \leq h_1 - 1 - \Lambda. \end{aligned} \tag{23}$$

Here all numbers in exponentials must be non-negative, and q is an integer which labels the multiplicity of a repeated pseudo angular momentum Λ for a given partition $[h_1 h_2]$ of $U(3)$. These multiple states of equal pseudo angular momentum are indexed by q and linearly independent, but not yet orthogonal. Orthogonality must be achieved by standard matrix methods. The permutation group $S(4)$ acting on relative coordinates is a subgroup of the pseudo rotation group $SO(3)$. The multiplicity of its representations, see Table 1, was given for all orbital partitions f of 4 particles in [14]. The polynomials eq. (23) have the maximum component Λ of the pseudo angular momentum. Lowering of the component is achieved by applying the first order lowering differential operator

$$\begin{aligned} \Lambda_- &= \Lambda_1 - i\Lambda_2 = z_-^1 \partial_0^1 - 2z_0^1 \partial_+^1 + z_-^2 \partial_0^2 - 2z_0^2 \partial_+^2, \\ \Lambda_3 &= z_+^1 \partial_+^1 - z_-^1 \partial_-^1 + z_+^2 \partial_+^2 - z_-^2 \partial_-^2. \end{aligned} \tag{24}$$

Λ^-	$[1^4]$	$[211]$	$[22]$	$[31]$	$[4]$	$\Lambda^\pi[1^4]$	$\Lambda^\pi[4]$
Λ^+	$[4]$	$[31]$	$[22]$	$[211]$	$[1^4]$		
0	1					0^-	0^+
1				1			
2		1	1				
3		1		1	1	3^+	3^-
4	1	1	1	1		4^-	4^+
5		1	1	2			
6	1	2	1	1	1	6^+6^-	6^-6^+
7		2	1	2	1	7^+	7^-
8	1	2	2	2		8^-	8^+
9	1	2	1	3	1	9^+9^-	9^-9^+
10	1	3	2	2	1	10^-10^+	10^+10^-
11		3	2	3	1	11^+	11^-
12	2	1	1	1	1	$(12^-)^212^+$	$(12^+)^212^-$
13	1	1	1	2	1	13^-13^+	13^+13^-
14	1	2	2	1	1	14^-14^+	14^+14^-
15	1	2	1	2	2	$15^-(15^+)^2$	$15^+(15^-)^2$
16	1	2	2	2	1	16^-16^+	16^+16^-
17	1	2	2	3	1	17^-17^+	17^+17^-
18	2	3	2	2	2	$(18^-)^2(18^+)^2$	$(18^+)^2(18^-)^2$
19	1	3	2	3	2	$19^-(19^+)^2$	$19^+(19^-)^2$
20	2	3	3	3	1	$(20^-)^220^+$	$(20^+)^220^-$
21	2	3	2	4	2	$(21^-)^2(21^+)^2$	$(21^+)^2(21^-)^2$
22	2	4	3	3	2	$(22^+)^2(22^-)^2$	$(22^-)^2(22^+)^2$
23	1	4	3	4	2	$23^-(23^+)^2$	$23^+(23^-)^2$
24	3	2	2	2	2	$(24^-)^3(24^+)^3$	$(24^+)^2(24^-)^2$

Table 1: Multiplicity of orbital partitions from [KM66] for given values $0 \leq \Lambda \leq 24$.

Finally we can also lower the angular momentum L from its maximum value $L = (h_1 - h_2)$ in steps of 2 by application of the angular momentum operators

$$\begin{aligned}
L^3 &= z_1^+ \partial_1^+ - z_1^- \partial_1^- + z_2^+ \partial_2^+ - z_2^- \partial_2^- + z_3^+ \partial_3^+ - z_3^- \partial_3^-, \\
L^- &= z_1^- \partial_1^+ + z_2^- \partial_2^+ + z_3^- \partial_3^+, \\
L^+ &= z_1^+ \partial_1^- + z_2^+ \partial_2^- + z_3^+ \partial_3^-.
\end{aligned} \tag{25}$$

3.3 From pseudo angular momentum Λ to orbital partitions f .

The orbital partitions [31], [4] do not apply for electrons with spin $s = \frac{1}{2}$. The entries for higher values of Λ than given in Table 1 are found by the recursive methods from [14] eq. (6.8).

4 States of four electrons.

A full orbital 4-particle state is characterized by the quantum numbers

$$|\alpha^4\rangle \equiv |\alpha^4 N, [h_1 h_2], \Lambda, L, f r\rangle, \quad (26)$$

where r ranges over the orbital Young tableaux of the diagram f . The total spin S is determined by antisymmetry and by the orbital partition f , see section 2.

4.1 Four electrons, $S=2$.

The orbital state has partition $f = [1111]$ of dimension $|[1111]| = 1$. The operator eq. 7 applied to the initial state $|\alpha^4\rangle$ becomes

$$|\alpha^4, [1111]\rangle = \sum_p T(p) |\alpha^4\rangle (-1)^p, \quad (27)$$

where $(-1)^p$ is the sign of the permutation p , +1 for even and -1 for odd permutations.

4.2 Four electrons, $S=1$.

The orbital partition is $f = [211]$ of dimension $|[211]| = 3$. The three Young diagrams (written for simplicity in rectangular frames) read

$$r_1 = \begin{bmatrix} 1 & 2 \\ 3 & \\ 4 & \end{bmatrix}, \quad r_2 = \begin{bmatrix} 1 & 3 \\ 2 & \\ 4 & \end{bmatrix}, \quad r_3 = \begin{bmatrix} 1 & 4 \\ 2 & \\ 3 & \end{bmatrix}. \quad (28)$$

Assume that the initial state $|\alpha^4[211]r_1\rangle$ has been generated by application of a Young operator eq.7. We find the two partner states of $|\alpha^4[211]r_1\rangle$ by the operator relations eq 11 and the axial distances,

$$\begin{aligned} |\alpha^4[211]r_2\rangle &= |\alpha^4[211]r_1\rangle \sqrt{\frac{1}{3}} + T(2,3) |\alpha^4[211]r_1\rangle \sqrt{\frac{4}{3}}, \quad \tau_{23}(r_1) = -2, \\ |\alpha^4[211]r_3\rangle &= |\alpha^4[211]r_2\rangle \sqrt{\frac{1}{8}} + T(3,4) |\alpha^4[211]r_2\rangle \sqrt{\frac{9}{8}}, \quad \tau_{34}(r_2) = -3. \end{aligned} \quad (29)$$

4.3 Four electrons, $\mathbf{S}=0$.

The orbital partition is $f = [22]$ of dimension $|[22]| = 2$. The two Young diagrams read

$$r_1 = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, r_2 = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}. \quad (30)$$

Again we generate the initial orbital state $|\alpha^4[22]r_1\rangle$ by application of a Young operator eq. 7. We find the second state by the operator relation and the axial distance

$$|\alpha^4[22]r_2\rangle = |\alpha^4[22]r_1\rangle\sqrt{\frac{1}{3}} + T(2, 3)|\alpha^4[22]r_1\rangle\sqrt{\frac{4}{3}}, \quad \tau_{23}(r_1) = -2. \quad (31)$$

5 Relative tetrahedral coordinates for $n = 4$ electrons.

Since we are dealing with particle-particle interactions, the cm vector is not affected, the total momentum is conserved, and the system is amenable to a description in relative coordinates. A standard choice are the Jacobi relative coordinates

$$\begin{aligned} \dot{\eta} &= Jz, \\ \dot{\eta}_1 &= \sqrt{\frac{1}{2}}(z_1 - z_2), \\ \dot{\eta}_2 &= \sqrt{\frac{1}{6}}(z_1 + z_2) - 2z_3, \\ \dot{\eta}_3 &= \sqrt{\frac{1}{12}}(z_1 + z_2 + z_3) - 3z_4. \end{aligned} \quad (32)$$

In [14] there was used a particular tetrahedral set of three doubledot relative coordinates. This set has the virtue that under the application of any permutation these relative coordinates are at most permuted, eq. 34. The transformation properties of the doubledot coordinates are summarized in [14] Table 3. The relative tetrahedral coordinates $\ddot{\eta}$ from [14], but now enumerated in the order of [9] for $n = 4$, are

$$\begin{aligned} \eta &= Qz, \\ \eta_1 &= \frac{1}{2}(z_1 + z_2 - z_3 - z_4) = \ddot{\eta}_3, \\ \eta_2 &= \frac{1}{2}(z_1 - z_2 + z_3 - z_4) = \ddot{\eta}_1, \\ \eta_3 &= \frac{1}{2}(z_1 - z_2 - z_3 + z_4) = \ddot{\eta}_2. \end{aligned} \quad (33)$$

It is found from [14], Table 3, that the tetrahedral coordinates eq. 33 have extremely simple matrix transformations under the generating transpositions (1, 2), (2, 3), (3, 4):

$$\begin{aligned} T^\eta(1, 2) \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}, \\ T^\eta(2, 3) \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix} &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}, \\ T^\eta(3, 4) \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}. \end{aligned} \quad (34)$$

The relative coordinates in Gusev [9] extend the tetrahedral coordinates eq. 33 to $n > 4$ particles. See Appendix B for their transforms under permutations.

We give now a first example of the polynomial state construction in the tetrahedral coordinates eq. 33 for the lowest excitation $N = 3$, $[h_1 h_2] = [30]$, $\Lambda = 3$, $f = [211]$ with spin $S = 1$ and the orbital Young tableaux r_1, r_2, r_3 of eq. 18:

$$\begin{aligned} |\alpha^4[211]r_1\rangle &= 2\sqrt{\frac{2}{3}}(\eta_2 - \eta_3)(\eta_2\eta_3 + \eta_1\eta_1), \\ |\alpha^4[211]r_2\rangle &= \frac{2}{3}\sqrt{2}(\eta_2 + \eta_3)(-\eta_1\eta_1 + \eta_2\eta_3 - 2\eta_1(\eta_2 - \eta_3)), \\ |\alpha^4[211]r_3\rangle &= \frac{4}{3}(\eta_2 + \eta_3)(\eta_1 - \eta_2)(\eta_3 + \eta_1). \end{aligned} \quad (35)$$

6 From matrix elements of the Coulomb interaction to the energy level structure.

With the polynomial states for a specific set of quantum numbers at hand, we proceed to evaluate the various parts of the four-electron Hamiltonian in the presence of a magnetic field B perpendicular to the (x, y) plane,

$$H = \sum_{i=1}^4 \frac{p_{x,i}^2 + p_{y,i}^2}{2m^*} + \frac{1}{2}m^*\Omega^2(x_i^2 + y_i^2) - \omega_L L_{z,i} + \sum_{i < j} \frac{e^2}{4\pi\epsilon_0\epsilon\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}}, \quad (36)$$

with the Larmor frequency $\omega_L = eB/(2m^*)$, the effective mass m^* and the combined frequency $\Omega^2 = \omega_0^2 + \omega_L^2$ due to an external confinement potential $V(x, y) = \frac{1}{2}m^*\omega_0^2(x^2 + y^2)$. In all following expressions we work within the symmetric gauge, which allows one to express the uniform magnetic field in terms of two-dimensional

oscillator excitations [13, 2]. The resulting four particle Hamiltonian is readily decomposed into cm and relative parts in the plane perpendicular to the magnetic field direction. Without the Coulomb part it resembles the addition of 2D oscillator systems with frequencies Ω . The magnetic field induces an angular-momentum dependent energy shift and the non-interacting eigenenergies read

$$E_{\text{cm}}(N_{\text{cm}}, M_{\text{cm}}) = \hbar\Omega(2N_{\text{cm}} + 1 + |M_{\text{cm}}|) - \hbar\omega_L M_{\text{cm}}, \quad (37)$$

$$N_{\text{cm}} = 0, 1, 2, \dots, M_{\text{cm}} = 0, \pm 1, \pm 2, \dots \quad (38)$$

$$E_{\text{rel}}(n_{\text{rel}}, m_{\text{rel}}) = \sum_{i=1}^3 \hbar\Omega(2n_{i,\text{rel}} + 1 + |m_{i,\text{rel}}|) - \hbar\omega_L m_{i,\text{rel}} \quad (39)$$

$$n_{\text{rel}} = 0, 1, 2, \dots, m_{\text{rel}} = 0, \pm 1, \pm 2, \dots \quad (40)$$

where we followed Fock's notation. In terms of the excitations n_i^\pm these quantum-numbers read

$$m_{i,\text{rel}} = n_i^+ - n_i^-, \quad 2n_i = n_i^+ + n_i^- - |n_i^+ - n_i^-| \quad (41)$$

The total energy is given by the addition of cm and relative parts

$$E_{\text{tot}} = E_{\text{cm}}(N_{\text{cm}}, M_{\text{cm}}) + E_{\text{rel}}(n_{\text{rel}}, m_{\text{rel}}) + E_{\text{rel,Coulomb}}. \quad (42)$$

For the evaluation of the Coulomb interaction we express the states as polynomials in the Jacobi relative vectors. There is, independent of the cm coordinate, a direct linear matrix transformation from relative tetrahedral to Jacobi vectors obtained from eqs. 32, 33, which for short we denote as

$$\dot{\eta} = JQ^{-1}\eta. \quad (43)$$

The first Jacobi vector from eq. 32 is the relative vector between particles 1,2 and according to eq. 8 it suffices to compute the full Coulomb interaction.

In the relative-coordinate polynomials the dimensionless Coulomb interaction reads

$$V_{\text{Coulomb}} = 6 \frac{\kappa}{\sqrt{2}\dot{\eta}}, \quad \kappa = \frac{e^2}{4\pi\epsilon_0\epsilon} \frac{m^*}{\hbar^2} \sqrt{\frac{\hbar}{m^*\Omega}}, \quad (44)$$

where the factor $4(4-1)/2 = 6$ arises from the number of pairs for the two-body operator in eq. 8.

The Coulomb matrix element between two states expressed in the three Jacobi vectors becomes

$$\begin{aligned} & \langle n_1^+ n_1^- n_2^+ n_2^- n_3^+ n_3^- | V_{\text{Coulomb}} | m_1^+ m_1^- m_2^+ m_2^- m_3^+ m_3^- \rangle \\ &= \delta(n_2^+, m_2^+) \delta(n_3^+, m_3^+) \delta(n_2^-, m_2^-) \delta(n_3^-, m_3^-) \delta(\sum_{i=1}^3 (n_i^+ - n_i^-), \sum_{i=1}^3 (m_i^+ - m_i^-)) \\ & \quad \times \delta(n_1^+ - n_1^-, m_1^+ - m_1^-) V_{\text{C}}(\min[n_1^+, n_1^-], \min[m_1^+, m_1^-], |n_1^- - n_1^+|), \end{aligned} \quad (45)$$

with

$$V_C(n, n', m) = \frac{\kappa\pi(-1)^{n+n'}\Gamma(|m|+\frac{1}{2})}{\sqrt{2}\Gamma(1/2-n)\Gamma(1+n)\Gamma(1/2-n')\Gamma(1+n')} \sqrt{\frac{n!}{(|m|+n)!}} \sqrt{\frac{n'!}{(|m|+n')!}} {}_3F_2\left(-n, -n', |m| + \frac{1}{2}; \frac{1}{2} - n, \frac{1}{2} - n'; 1\right) \quad (46)$$

We construct for a given set of relative-coordinate excitations all relative-coordinate states q_i and express each state $q_i(\dot{\eta}_1, \dot{\eta}_2, \dot{\eta}_3)$ as sum of polynomials in Jacobi coordinates with exponents $n_{i,j}^\pm$

$$q_i = \sum_{j=1} a_{i,j} \dot{\eta}_1^{n_{1,i,j}^+} \dot{\eta}_1^{n_{1,i,j}^-} \dot{\eta}_2^{n_{2,i,j}^+} \dot{\eta}_2^{n_{2,i,j}^-} \dot{\eta}_3^{n_{3,i,j}^+} \dot{\eta}_3^{n_{3,i,j}^-}. \quad (47)$$

Then the interaction matrix is given by

$$M_C(q_i, q_k) = \sum_{j,m} a_{i,j} a_{k,m}^* \langle n_{1,i,j}^+ n_{1,i,j}^- n_{2,i,j}^+ n_{2,i,j}^- n_{3,i,j}^+ n_{3,i,j}^- | V_C | n_{1,k,m}^+ n_{1,k,m}^- n_{2,k,m}^+ n_{2,k,m}^- n_{3,k,m}^+ n_{3,k,m}^- \rangle. \quad (48)$$

The Coulomb interaction does not connect states with different angular momenta and so the blocks of states (S, f) fall into subblocks labelled by (S, f, m_{rel}) . However, different excitations of the relative oscillator are coupled by the Coulomb interaction. The addition of the relative oscillators, including the Coulomb interaction is given by diagonalization of the matrix

$$M_{\text{rel}}(q_i, q_k) = M_C(q_i, q_k) + \delta_{ik} \hbar\Omega \sum_{i=1}^3 (1 + n_i^+ + n_i^-) \quad (49)$$

If we augment the relative eigenvalues with the analytic results for the cm energies, we are in a position to compare the results with the configuration-interaction methods using Slater determinantes of single-particle states.

6.1 Spin $S = 2$ and the Laughlin state.

As first example we discuss four electrons in a magnetic field with $\omega_0 = 0$ and the maximum spin state $S = 2$. Due to the maximum spin state with all spins coinciding, the orbital state must be completely antisymmetric, $f = 1^4$. We choose $n_{\text{rel}} = 18$, $m_{\text{rel}} = 18$ (corresponding to the lowest Landau level) and the basis set consists of seven states with pseudo angular momenta $\Lambda = 6, 10, 12, 14, 16, (18)^2$. The corresponding SACI basis set restricted to the lowest Landau level contains already additional 27 spurious states due to the admixing of cm excitations.

It is instructive to see which linear combination of the seven non-spurious states yields the Laughlin state, which is also free of any cm excitations. The Laughlin

1.8466	2.1596	2.3833	2.5451
2.0012	2.2136	2.3899	2.6327
2.0217	2.2529	2.4127	2.6597
2.0284	2.2589	2.4453	2.7362
2.0704	2.2959	2.4534	2.7974
2.1042	2.3132	2.4722	2.9591
2.1223	2.3133	2.4997	3.1498
2.1265	2.3215	2.5245	
2.1531	2.3832	2.5441	

Table 2: List of 34 SACI Coulomb eigenvalues ($\kappa = 1$) in units of $\hbar\Omega$ for $S = 2$ obtained by diagonalization of the Slater determinants of the 34 single-particle product states $\prod_{i=1}^4 |\phi(0, l_i)\rangle$ yielding $L = \sum_{i=1}^4 l_i = 18$ within the lowest Landau level. The entries in boldface indicate the seven states with the cm oscillator in the ground state obtained by the polynomial method described in the text for the lowest Landau level ($n_{\text{rel}} = m_{\text{rel}} = 18$), while the remaining 27 eigenvalues correspond to spurious states.

antisymmetric trial function at filling factor $1/3$ is written in terms of the single-particle states [24]

$$\psi_{1/3} = [(z_1^+ - z_2^+)(z_1^+ - z_3^+)(z_1^+ - z_4^+)(z_2^+ - z_3^+)(z_2^+ - z_4^+)(z_3^+ - z_4^+)]^3. \quad (50)$$

The Coulomb interaction with $\kappa = 1$ yields an expectation value of $1.8535 \hbar\Omega$ for the $\psi_{1/3}$ state, slightly above the lowest eigenvalue $1.8466 \hbar\Omega$ obtained by diagonalization of the Coulomb matrix M_C within the seven state basis set.

6.2 Intrusion of cm excitation for the spin $S = 0$ case.

As second example, we consider the case $f = [22]$ with total angular momentum $L_{\text{tot}} = M_{\text{cm}} + m_{\text{rel}} = 0$, $\omega_L = 0$. The relative-coordinate method allows one to decompose the problem into irreducible blocks which are separately diagonalized. In Fig. 1 the possible combinations of relative and cm angular momenta and excitations are depicted, which result in $L_{\text{tot}} = 0$. If we consider all basis states with $E_{\text{total}}^{\kappa=0} \leq 10\hbar$ the Slater-determinantal SACI methods yields 42 basis states. The irreducible group-theoretical approach yields decomposes these states into a block-diagonal basis sets of size 14 ($m_{\text{rel}} = 0$), 5 ($m_{\text{rel}} = \pm 1$), and 4 ($m_{\text{rel}} = \pm 2$), marked by green, red and blue arrows in Fig. 1. The additional 19 states (8 non-degenerate) of the SACI basis are all spurious states with $N_{\text{cm}} > 0$.

Besides the smaller block sizes, another observation is that by fixing a cut-off energy in terms of $E_{\text{total}}^{\kappa=0}$ in the configuration-interaction method, copies of basis elements

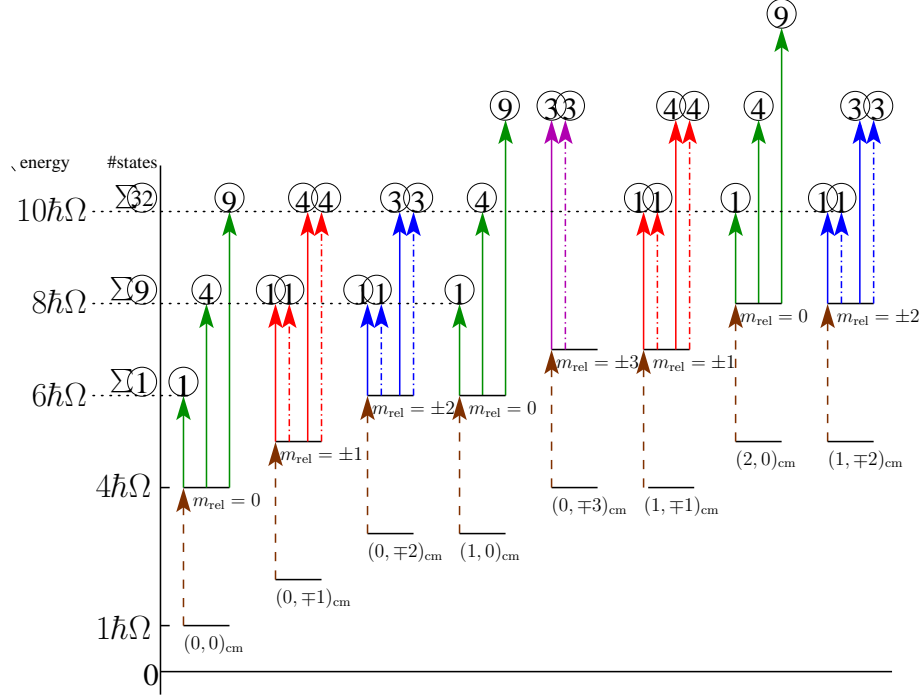


Figure 1: Decomposition of the total angular state $L_{\text{tot}} = 0$ for spin $S = 0$ for four electrons into relative-coordinate building blocks. Excitations of cm angular momentum M_{cm} have to be combined with $m_{\text{rel}} = -M_{\text{cm}}$ values, which leads to a redundancy of interaction matrix elements. For instance, the 32 states at total energy $E = 10\hbar\Omega$ can be broken down into three copies of relative-coordinate states (color coded). Each ladder starts with a cm state denoted by $(N_{\text{cm}}, M_{\text{cm}})_{\text{cm}}$, to which the zero-point energy 3 of the relative-coordinate oscillators is added. The numbers in circles denote the number of relative-coordinate states with an excitation corresponding to the length of each arrow.

with the same relative excitation and angular momentum are included but with varying number of excitations. For instance, while the $m_{\text{rel}} = 0$ state is included in the energy levels $E_{\text{total}}^{\kappa=0} \leq 10\hbar$ with three excitation levels $N = 2, 4, 6$ on top of the $(N_{\text{cm}} = 0, M_{\text{cm}} = 0)_{\text{cm}}$ state, it enters for $(1, 0)_{\text{cm}}$ with only 2 excited levels and at $(2, 0)_{\text{cm}}$ only with its ground state.

Fig. 2 demonstrates how the uneven inclusion of excited relative-coordinate states in the SACI basis results in a skewed eigenvalue spectrum of the SACI method and does not allow one to identify cm copies by scanning for eigenvalues spaced by the cm excitation $\hbar\Omega$. In contrast, the separation of relative and cm states in the group-theoretical approach preserves the exact spacing of the cm sets and the diagonalization only affects the subspace of relative-coordinate states, as required.

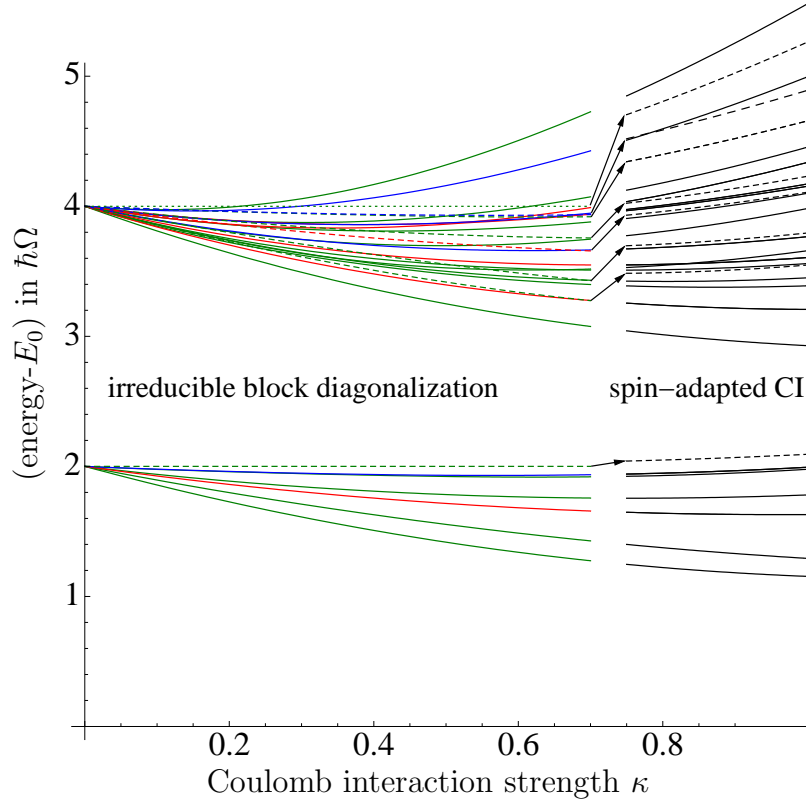


Figure 2: Evolution of the lowest 42 eigenenergies of a four electron quantum dot ($\omega_L = 0$) as function of the Coulomb interaction strength κ . The lowest eigenvalue E_0 has been subtracted. The left curves ($\kappa \leq 0.7$) are obtained by the irreducible approach using relative-coordinates and provide better converged values than the the spin-adapted configuration interaction method (SACI) (right curves $\kappa > 0.75$). The inaccuracies of the determinantal SACI method (upward arrows) affect all spurious states with $N_{\text{cm}} > 0$ (dashed and dotted lines).

Similar results apply to the spin $S = 1, 2$ states.

In particular SACI yields less-accurate eigenvalues at the higher eigenenergies (see the upward pointing arrows in Fig. 2), while the group-theoretical approach preserves the accuracy by combining the low-lying relative coordinate eigenvalues with the exact cm excitation energy. Table 3 gives the lowest eigenenergy for the $m_{\text{rel}} = 0$ state as function of relative coordinate excitation, which approaches the exact ground state eigenenergy with increasing basis size.

maximal relative excitation	2	4	6	8	10
basis size irred. rep.	1	5	14	35	74
SACI basis size	1	10	42	145	405
lowest eigenenergy	11.483	10.685	10.592	10.555	10.539

Table 3: Lowest eigenenergy for the $m_{\text{rel}} = 0$ case, Coulomb interaction $\kappa = 1$, $\omega_L = 0$ in units of $\hbar\Omega$. For the lowest eigenvalue, SACI and the irreducible block diagonalization yield identical results upon inclusion of the same maximal relative excitation, however the SACI basis set is substantially larger due to the inclusion of spurious states.

7 Summary of the group theoretical approach to construct the *cm* free basis.

The construction of the basis set of relative coordinate polynomials for n electrons entailed the following steps:

- (1) Spin, partition: Given the number n of electrons, we determine the possible spins S , orbital partitions f and angular momenta L . The state space falls into independent and orthogonal subspaces labeled by (S, f, L) . Steps (1-7) work for $n=4$. For $n > 4$ and steps (4-7) an extended analysis needs to be developed, some results are given in the appendices.
- (2) Unitary quantum numbers: We provide the orbital quantum numbers of the system. For a maximal relative oscillator excitation N we list the unitary partitions $[h_1 h_2]$, $h_1 + h_2 = N$ for the groups $U(2) \times U(n-1)$. A restriction to the lowest Landau level LLL with $[h_1 h_2] \rightarrow [N0]$ greatly simplifies the analysis.
- (3) Angular momenta: The unitary partition $[h_1, h_2]$ from $U(2) > O(2)$ fixes the ladder of angular momenta L from the maximum value $L_{\text{max}} = h_1 - h_2$ in steps of 2 down to 0 or 1 and provides the final blocks (S, f, L) .
- (4) Pseudo angular momentum and partition: The pseudo angular momentum Λ is obtained from $[h_1, h_2]$ by the representation theory of the rotation subgroup in $O(n-1) < U(n-1)$. For $n = 4$, any fixed pseudo angular momentum Λ yields from [14] p. 260 a precise list of possible orbital partitions f . Multiple values of pseudo angular momentum yield linearly independent polynomials.
- (5) State polynomials: Given this list of quantum numbers, we construct state polynomials in relative coordinates. The initial polynomial is known from [3]. The component of pseudo angular momentum and of total angular momentum are lowered independently.
- (6) Young tableau: For the known orbital partitions f , by applying permutation operators we project states with definite Young tableau.
- (7) Coulomb interaction and energies: For state polynomials in a block (S, f, L) , we

isolate the first Jacobi vector in bra and a ket states, evaluate the matrix elements of the Coulomb interaction, determine the hamiltonian matrix, diagonalize it and find the eigenstates of relative motion.

8 Conclusion.

The study of the four-electron quantum-dot with Coulomb interactions in the relative-coordinate basis elucidates and overcomes some of the problems inherent in the commonly used configuration interaction methods such as SACI [27, 28]: If the cm excitations, as in determinantal state space, cannot be separated, a large cloud of spurious cm excited states, augmented by spurious angular momenta, intrudes the variational state space and obscures the variational energy spectrum reflecting the Coulomb interaction. Within SACI, higher eigenenergies are distorted by the Coulomb interaction and a loss in accuracy is seen, which can be avoided by the separation of the relative and cm coordinates. This allows one to construct polynomial states with labels from representations of unitary and rotation groups and to diagonalize the Coulomb-interaction part in smaller subblocks. Our approach opens a clear view on the energy spectrum as shown in Figs. 1 and 2 and preserves the exact ladder spacing $\hbar\Omega$ of cm copies of the relative coordinates variational subspace. By increasing the basis size with respect to the relative excitations, the eigenenergies and eigenvectors obtained by diagonalization converge toward the exact eigenstates of the system.

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9 Appendix A: Alternative state analysis by use of the subgroup $D_{2d} < S(4)$.

An independent view on orbital basis states for 4 electrons under permutations arises by use of the subgroup $D_{2d} < S(4)$ from [14]. This method can be extended to higher excitations. It allows in Tables 7,8 to identify states of permutational symmetry for any pseudo angular momentum almost without projection. We use (λ, μ) to denote a standard state of pseudo angular momentum λ with component μ , $\kappa = 0, 1$ for parity, and $\rho = \pm 1$ with the states defined in eq. 51. As mentioned in [14] p. 263, the group D_{2d} is the largest subgroup of $S(4)$ that leaves invariant the double-dot \vec{e}_3 axis up to a reflection. With the Frobenius multiplicity expression we assign from the characters of D_{2d} , Table 4, in Table 6 the reduction of IR f of $S(4)$ to those of D_{2d} . The numbers $(\kappa\rho\epsilon)$ are taken from [14] and used in Table 4. They determine the irreducible bases of representation of D_{2d} but from Table 6 also basis states of permutational symmetry. The basis states $[31]_3$ and $[211]_3$ are unique, and so their partner states may be derived by the ladder procedure 11. The basis functions for $f = [31], [211]$ here transform like the doubledot representation. By [14] eqs. (6.1, 6.9) we can always return from the doubledot basis to the Jacobi basis. The basis states of $f = [22]$ can be separated from the bases of $f = [4]$ and $f = [1^4]$ by projection.

We fix for the moment the labels κ, ϵ and introduce $\rho = \pm 1$ in eq. 51. Motivated by [14], but independent of it, we redefine two new linear combinations of spherical harmonics [6] (2.5.7) by

$$\begin{aligned} \rho = 1 : |1(\lambda, \mu)\rangle &= g_\mu[|(\lambda, \mu)\rangle + |(\lambda, -\mu)\rangle(-)^{\lambda+\mu}], \mu \geq 0, \\ \rho = -1 : |-1(\lambda, \mu)\rangle &= i^{-1}g_\mu[|(\lambda, \mu)\rangle - |(\lambda, -\mu)\rangle(-)^{\lambda+\mu}], \mu > 0. \end{aligned} \quad (51)$$

These states by consulting [14] Table 3 may be shown to be orthogonal eigenstates of the permutation operator $T((1, 4)(2, 3))$ with eigenvalue $\rho = \pm 1$, which from [14] Fig 1 reverses the axis \vec{e}_3 . States characterized by (κ, ϵ, ρ) we show to belong to irreps of the subgroup D_{2d} . For the proof we employ the class operators [14], which are group operators $T(g)$ summed over a class of equivalent group elements, and commute with any group operator. The five class operators Ki [14] of the group D_{2d} , written as sums of permutation operators from [14], Table 4 are

$$\begin{aligned} K1 &= T(e), \\ K2 &= T((3, 4)(1, 2)), \\ K3 &= T(1, 3, 2, 4) + T(4, 2, 3, 1), \\ K4 &= T((1, 3)(2, 4)) + T((1, 4)(2, 3)), \\ K5 &= T(1, 2) + T(3, 4). \end{aligned} \quad (52)$$

<i>irrep</i>	E	S_4	C_2	$2C'_2$	$2\sigma_d$
$1 : A_1$	1	1	1	1	1
$2 : A_2$	1	1	1	-1	-1
$3 : B_1$	1	-1	1	1	-1
$4 : B_2$	1	-1	1	-1	1
$5 : E$	2	0	-2	0	0

Table 4: Characters of the five IR 1, ..., 5 of D_{2d} for its five classes in the irreducible representations.

By use of the representation matrices of permutations we express the class operators eq. 52 in matrix form, Table 5. The matrix forms depend on the chosen representation, and we make convenient choices: For the representations $D^{[31]}$ and $D^{[211]}$, $D^{[211]}(i, j) = ID^{[31]}((i, j))$ we use the basis eq. 33 of $\dot{\eta}_j$, for the representation $D^{[22]}$ the Young representation [10] p. 226. By virtue of these choices we find: All class operators eq. 52 have diagonal representations, see Table 5. This proves:

Prop: All basis states of the irreps of the subgroup D_{2d} in the chosen representations are basis states of irreducible representations of the bigger group $S(4)$.

This remarkable result allows in Table 6, up to certain ambiguities, to almost avoid the use and projection with Young operators for the bigger group $S(4)$. In Tables 7,8 we use it in relation with the full scheme of groups including $SU(3) > O(3, R)$ and subgroups to assign orbital symmetry to the oscillator states.

Of two states separated by $|$, one and only one can belong to the listed tableau. The states $[4], [1^4]$ are identified as eigenstates under the transposition $T(2, 3)$ with eigenvalue ± 1 respectively. If a state is not reproduced under $T(2, 3)$, it necessarily belongs to $f = [22]$ and spin $S = 0$. We conclude that the states eq. 51 yield all the bases of the orbital Young tableaux.

class	$D^{[4]}(Ki)$	$D^{[31]}(Ki)$	$D^{[211]}(Ki)$	$D^{[22]}(Ki)$	$D^{[1^4]}(Ki)$
$K1$	$\begin{bmatrix} 1 \end{bmatrix}$	$\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$	$\begin{bmatrix} 1 \end{bmatrix}$
$K2$	$\begin{bmatrix} 1 \end{bmatrix}$	$\begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & & \\ & -1 & \\ & & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$	$\begin{bmatrix} 1 \end{bmatrix}$
$K3$	$\begin{bmatrix} 2 \end{bmatrix}$	$\begin{bmatrix} & & \\ & & \\ & & -2 \end{bmatrix}$	$\begin{bmatrix} & & \\ & & \\ & & 2 \end{bmatrix}$	$\begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$	$\begin{bmatrix} -2 \end{bmatrix}$
$K4$	$\begin{bmatrix} 2 \end{bmatrix}$	$\begin{bmatrix} & & \\ & & \\ & & -2 \end{bmatrix}$	$\begin{bmatrix} & & \\ & & \\ & & -2 \end{bmatrix}$	$\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$	$\begin{bmatrix} 2 \end{bmatrix}$
$K5$	$\begin{bmatrix} 2 \end{bmatrix}$	$\begin{bmatrix} & & \\ & & \\ & & 2 \end{bmatrix}$	$\begin{bmatrix} & & \\ & & \\ & & -2 \end{bmatrix}$	$\begin{bmatrix} 2 & \\ & -2 \end{bmatrix}$	$\begin{bmatrix} -2 \end{bmatrix}$

Table 5: Diagonal matrix representations $D^f(Ki)$ for partitions $f = [4], [31], [211], [22], [1^4]$, non-zero entries only, of the class operators $K1, \dots, K5$ eq. 52 of $D_{2d} < S(4)$.

κ	ϵ	$\rho = 1$	$\rho = -1$
0	+1	$[22]_2 [4]$	$[211]_3$
0	-1	$[22]_1 [1^4]$	$[31]_3$
0	0	$[31]_1 [211]_1$	$[31]_2 [211]_2$
1	+1	$[22]_1 [1^4]$	$[31]_3$
1	-1	$[22]_2 [4]$	$[211]_3$
1	0	$[211]_1 [31]_1$	$[211]_2 [31]_2$

Table 6: Basis states for all orbital partitions f of $S(4)$ in correspondence to irreducible representations of the group D_{2d} indexed by the labels of parity $\kappa = 0, 1$, eigenvalue $\rho = 1, -1$ eq. 51, and $\epsilon := (i^{|\mu|} + i^{-|\mu|})/2 = 1, 0, -1$, from caption Table 8, compare [14] p.267, Table 5.

N^π	Λ^π	$ \mu $	κ	ϵ	$\rho = 1$	$\rho = -1$	(λ', μ')	Λ^π	f
0^+	0^+	0	0	1	$[4]^+$	—	$(0, 0)$	0^+	$[4]$
1^-	1^-	1	1	0	$[31]1^+$	$[31]2^+$	$(1, 0)$	1^-	$[31]$
		0	1	1	—	$[31]3^+$			
2^+	2^+	2	0	-1	$[22]1^+$	$[31]3^+$	$(2, 0)$	2^+	$[31][22]$
		1	0	0	$[31]1^+$	$[31]2^+$			
		0	0	1	$[22]2^+$	—			
	1^+	1	0	0	$[211]1^+$	$[211]2^+$	$(0, 1)$	1^+	$[211]$
		0	0	1	—	$[211]3^+$			
	0^+	0	0	1	$[4]^+$	—	$(2, 0)$	0^+	$[4]$
3^-	3^-	3	1	0	$[211]1 [31]1^*$	$[211]2 [31]2^*$	$(3, 0)$	3^-	$[211][31][4]$
		2	1	-1	$[4]^+$	$[211]3^+$			
		1	1	0	$[211]1 [31]1^*$	$[211]2 [31]2^*$			
		0	1	1	—	$[31]3^+$			
	2^-	2	1	-1	$[22]2^+$	$[211]3^+$	$(1, 1)$	2^-	$[211][22]$
		1	1	0	$[211]1^+$	$[211]2^+$			
		0	1	1	$[22]1^+$	—			
	1^-	1	1	0	$[31]1^+$	$[31]2^+$	$(3, 0), (1, 1)$	$(1^-)^2$	$[31]^2$
		0	1	1	—	$[31]3^+$			
4^+	4^+	4	0	1	$[22]2 [4]^*$	$[211]3^*$	$(4, 0)$	4^+	$[4][31][22][211]$
		3	0	0	$[31]1 [211]1^*$	$[31]2 [211]2^*$			
		2	0	-1	$[22]1^+$	$[31]3^+$			
		1	0	0	$[31]1 [211]1^*$	$[31]2 [211]2^*$			
		0	0	1	$[22]2 [4]^*$	$[211]3^*$			
	3^+	3	0	0	$[31]1 [211]1^*$	$[31]2 [211]2^*$	$(2, 1)$	3^+	$[31][211][1^4]$
		2	0	-1	$[1^4]$	$[31]3^+$			
		1	0	0	$[31]1 [211]1^*$	$[31]2 [211]2^*$			
		0	0	1	—	$[211]3^+$			
	2^+	2	0	-1	$[22]1^+$	$[31]3^+$	$(4, 0), (2, 1), (0, 2)$	$(2^+)^3$	$[31]^3[22]^3$
		1	0	0	$[31]1^+$	$[31]2^+$			
		0	0	1	$[22]2^+$	—			
	1^+	1	0	0	$[211]1^+$	$[211]2^+$	$(2, 1)$	1^+	$[211]$
		0	0	1	—	$[211]3^+$			
	0^+	0	0	1	$[4]^+$	—	$(4, 0), (0, 2)$	$(0^+)^2$	$[4]^2$

Table 7: continued on next table

N^π	Λ^π	$ \mu $	κ	ϵ	$\rho = 1$	$\rho = -1$	(λ', μ')	Λ^π	f
5^-	5^-	5	1	0	$[211]1 [31]1*$	$[211]2 [31]2*$	$(5, 0)$	5^-	$[211][22][31]^2$
		4	1	1	$[22]1+$	$[31]3+$			
		3	1	0	$[211]1 [31]1*$	$[211]2 [31]2*$			
		2	1	-1	$[22]2+$	$[211]3+$			
		1	1	0	$[211]1 [31]1*$	$[211]2 [31]2*$			
		0	1	1	$[22]1+$	$[31]3+$			
	4^-	4	1	1	$[1^4][22]1*$	$[31]3+$	$(3, 1)$	4^-	$[1^4][211][22][31]$
		3	1	0	$[211]1 [31]1*$	$[211]2 [31]2*$			
		2	1	-1	$[22]2+$	$[211]3+$			
		1	1	0	$[211]1 [31]1*$	$[211]2 [31]2*$			
		0	1	1	$[22]1 [1^4]*$	$[31]3+$			
	3^-	3	1	0	$[211]1 [31]1*$	$[211]2 [31]2*$	$(5, 0)(3, 1)(1, 2)$	$(3^-)^3$	$[211]^3[31]^3[4]^3$
		2	1	-1	$[4]+$	$[211]3+$			
		1	1	0	$[211]1 [31]1*$	$[211]2 [31]2*$			
		0	1	1	—	$[31]3+$			
	2^-	2	1	-1	$[22]2+$	$[211]3+$	$(3, 1)(1, 2)$	$(2^-)^2$	$[211]^2[22]^2$
		1	1	0	$[211]1+$	$[211]2+$			
		0	1	1	$[22]1+$	—			
	1^-	1	1	0	$[31]1+$	$[31]2+$	$(5, 0)(3, 1)(1, 2)$	$(1^-)^3$	$[31]^3$
		0	1	1	—	$[31]3+$			

Table 8: Permutational states combining D_{2d} with $SU(3, C)$ labels.

$N \leq 5$ total excitation/degree, Orbital 2D angular momentum range: $L = \lambda', \lambda' - 2, \dots, 1$ or 0. States marked + are unambiguous. Λ pseudo angular momentum with component μ , $\pi = \pm 1$ standard parity.

D_{2d} , columns 1-7 from [14]: $|\mu|$ absolute value of Λ 's component, $\kappa = 0, 1$ [14] parity, $\rho = \pm 1$ eigenvalue eq. 52 of pseudo-spherical state eq. 51. Vertical bars separate ambiguous choices marked by *, select one by ladder procedure. Note that labels depend only on Λ, κ .

$SU(3, C)$, columns 8-10 from [26],[14]: (λ', μ') standard irrep labels, Λ^π pseudo angular momentum [26] p.177 and parity π , f orbital partition of $S(4)$, multiplicity from [14] p.260.

10 Appendix B: Symmetrized relative coordinates for $n > 4$ electrons and their permutations.

The efficiency of the tetrahedral coordinates raises the question if similar relative coordinates exist for $n > 4$. As a generalization of the tetrahedral coordinates from [14], new symmetrized coordinates for n particles were proposed by Gusev et al [9]. The matrix that gives the n new coordinates $(\eta_0, \eta_1, \dots, \eta_{n-1})$ in terms of the old ones (x_1, x_2, \dots, x_n) reads

$$C = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & 1 & \dots & 1 & 1 \\ 1 & b & a & a & \dots & a & a \\ 1 & a & b & a & \dots & a & a \\ \cdot & \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ 1 & a & a & a & \dots & b & a \\ 1 & a & a & a & \dots & a & b \end{bmatrix}, \quad (53)$$

$$C = C^T, \quad C^{-1} = C, \quad C^2 = I,$$

$$a = [1 - \sqrt{n}]^{-1}, \quad b = a + \sqrt{n}.$$

The cm coordinate is included as η_0 . We shall explore the properties of these coordinates under the action of permutations. All permutations are generated by products of the $n - 1$ transpositions $(1, 2), (2, 3), \dots, (n - 1, n)$. We need the action of these transpositions on the new relative coordinates. We shall see in eq. 56 that under permutations $h \in S(n - 1)$ acting on particles $(2, 3, \dots, n)$ the symmetrized coordinates transform like single particle coordinates. So we focus on the remaining action $D^\eta(1, 2)$ of the first transposition $(1, 2)$ with respect to the new coordinates.

10.1 The example of $n = 5$ electrons.

For $n = 5$ we obtain for the linear action of the transposition $(1, 2)$ on the new coordinates

$$D^\eta(1, 2) = \frac{1}{5} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & b & a & a & a \\ 1 & a & b & a & a \\ 1 & a & a & b & a \\ 1 & a & a & a & b \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & b & a & a & a \\ 1 & a & b & a & a \\ 1 & a & a & b & a \\ 1 & a & a & a & b \end{bmatrix} \quad (54)$$

$$= \frac{1}{5} \begin{bmatrix} 5 & 1 + 3a + b & 1 + 3a + b & 1 + 3a + b & 1 + 3a + b \\ 1 + 3a + b & 2b + 3a^2 & a + b + 2a^2 + ab & a + b + 2a^2 + ab & a + b + 2a^2 + b^2 \\ 1 + 3a + b & a + b + 2a^2 + ab & 2a + 2a^2 + b^2 & 2a + a^2 + 2ab & 2a + a^2 + 2ab \\ 1 + 3a + b & a + b + 2a^2 + ab & 2a + a^2 + 2ab & 2a + 2a^2 + b^2 & 2a + a^2 + 2ab \\ 1 + 3a + b & a + b + 2a^2 + b^2 & 2a + a^2 + 2ab & 2a + a^2 + 2ab & 2a + 2a^2 + b^2 \end{bmatrix}$$

This matrix is symmetric and orthogonal by construction, its square is the unit matrix.

We compute from eqs.23,28,33 the numbers

$$\begin{aligned}
a &= -\frac{1}{4}[1 + \sqrt{5}], \quad b = -\frac{1}{4}[1 - 3\sqrt{5}], \\
(002300) &= 2b + 3a^2 = \frac{1}{8}[5 - \sqrt{5}], \\
(011201) &= a + b + 2a^2 + ab = \frac{5}{8}[-1 + \sqrt{5}], \\
(020210) &= 2a + 2a^2 + b^2 = \frac{5}{8}[5 - \sqrt{5}], \\
(020102) &= 2a + a^2 + 2ab = -\frac{5}{8}[3 + \sqrt{5}].
\end{aligned} \tag{55}$$

For $n = 5$, all the numbers and matrices can be decomposed into a rational part and a second part rational but proportional to $\sqrt{5}$. All these numbers form a module that closes under addition, multiplication and division, compare the example eq. 25. We give this decomposition in the following examples. A similar module decomposition applies for any n whose square root is not an integer.

$$\begin{aligned}
C &= A + \sqrt{5}B, \\
A &= \frac{1}{4} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & -1 & -1 & -1 \\ 0 & -1 & -1 & -1 & -1 \\ 0 & -1 & -1 & -1 & -1 \\ 0 & -1 & -1 & -1 & 3 \end{bmatrix}, \quad B = \frac{1}{4 \cdot 5} \begin{bmatrix} 4 & 4 & 4 & 4 & 4 \\ 4 & -1 & -1 & -1 & -1 \\ 4 & -1 & -1 & -1 & -1 \\ 4 & -1 & -1 & -1 & -1 \\ 4 & -1 & -1 & -1 & -1 \end{bmatrix}, \\
D^\eta(1, 2) &= A^\eta + \sqrt{5}B^\eta, \\
A^\eta &= \frac{1}{5 \cdot 8} \begin{bmatrix} 5 \cdot 8 & 0 & 0 & 0 & 0 \\ 0 & 5 & -5 & -5 & -5 \\ 0 & -5 & 25 & -15 & -15 \\ 0 & -5 & -15 & 25 & -15 \\ 0 & -5 & -15 & -15 & 25 \end{bmatrix}, \quad B^\eta = \frac{1}{5 \cdot 8} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 5 & 5 & 5 \\ 0 & 5 & -5 & -5 & -5 \\ 0 & 5 & -5 & -5 & -5 \\ 0 & 5 & -5 & -5 & -5 \end{bmatrix}.
\end{aligned} \tag{56}$$

We find with eq.55 from the values of a, b for $n = 5$,

$$1 + 3a + b = 0 \tag{57}$$

and so the product matrix eq.54 reduces to its diagonal 4×4 submatrix that involves only the relative coordinates $\eta_1, \dots, \eta_{n-1}$. This is always necessary, since the transposition $(1, 2)$ cannot affect the cm coordinate η_0 . For the other transpositions $(i, i + 1), i > 1$ we find the result

$$2 \leq i \leq (n - 1) = 4 : T(i, i + 1)\eta_{i-1} = \eta_i, \quad T(i, i + 1)\eta_i = \eta_{i-1} \tag{58}$$

So all transpositions $(i, i+1)$ in single particle coordinates $2, \dots, n$ act on the relative coordinates $(\eta_1, \eta_2, \dots, \eta_{n-1})$ like transpositions of relative coordinates which we denote as $T^\eta(i-1, i)$. We summarize eq. 56 in symbolic form as

$$T(i, i+1) \sim T^\eta(i-1, i), \quad i = 2, \dots, n-1. \quad (59)$$

The transposition $T(1, 2)$, missing in eq. 59, and acting on the symmetrized coordinates, is given by the matrix $D^\eta(1, 2)$ eq. 62.

10.2 Permutations of symmetrized relative coordinates for n electrons.

The results of the last subsection, in particular eq. 59 generalize to any n . Since the transpositions eq. 56 generate the subgroup $S(n-1)$, all permutations of particles $(2, \dots, n)$ are mapped by eq. 59 into permutations of the relative coordinates $(\eta_1, \dots, \eta_{n-1})$. The correspondence eq. 59 must be kept in mind when working with the new relative coordinates.

We could easily antisymmetrize a polynomial state wrt to the $(n-1)$ particles $2, 3, \dots, n$, but must augment the antisymmetrizer A^{n-1} to include particle 1, see the next section. In terms of the symmetric group, we have the subgroup $S(n-1)$ acting on particles $2, 3, \dots, n$. All elements $p \in S(n)$ can be written as $p = c_i h$ with $h \in S(n-1)$, multiplied by the n coset generators which may be chosen as transpositions $c_0 = e, c_i = (1, i), i = 2, \dots, n$. These coset generators can be rewritten as

$$(1, i) = (i, 2)(1, 2)(2, i), \quad i = 3, \dots, n, \quad (i, 2) \in S(n-1) \quad (60)$$

and so their matrices $D^\eta(1, i)$ acting on relative coordinates reduce to the element $D^\eta(1, 2)$ whose matrix we compute in eq. 59. The representations $D^\eta(i, 2), i = 2, \dots, n$ appearing in eq. 57 simply mean the interchange of two rows or two columns. So our main task is to give the generalization of eq. 54 for any n . We denote the matrix elements of $D^\eta(1, 2)$ for short by six integers

$$(n_0 n_1 n_2 n_3 n_4 n_5) \rightarrow (n_0 + n_1 a + n_2 b + n_3 a^2 + n_4 b^2 + n_5 ab), \quad (61)$$

$$a = [1 - \sqrt{n}]^{-1}, \quad b = a + \sqrt{n},$$

and obtain for the matrix representation in η -coordinates and general n the result

$$D^\eta(1, 2) = CD(1, 2)C^{-1} \quad (62)$$

$$= \frac{1}{n} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & . \\ 1 & b & a & a & a & . \\ 1 & a & b & a & a & . \\ 1 & a & a & b & a & . \\ 1 & a & a & a & b & . \\ . & . & . & . & . & . \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & . \\ 1 & 0 & 0 & 0 & 0 & . \\ 0 & 0 & 1 & 0 & 0 & . \\ 0 & 0 & 0 & 1 & 0 & . \\ 0 & 0 & 0 & 0 & 1 & . \\ . & . & . & . & . & . \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & . \\ 1 & b & a & a & a & . \\ 1 & a & b & a & a & . \\ 1 & a & a & b & a & . \\ 1 & a & a & a & b & . \\ . & . & . & . & . & . \end{bmatrix}$$

$$= \frac{1}{n} \begin{array}{|c|c|c|c|c|c|} \hline (n00000) & (1n-21000) & (1n-21000) & (1n-21000) & (1n-21000) & . \\ \hline (1n-21000) & (002n-200) & (011n-301) & (011n-301) & (011n-301) & . \\ \hline (1n-21000) & (011n-301) & (020n-310) & (020n-402) & (020n-402) & . \\ \hline (1n-21000) & (011n-301) & (020n-402) & (020n-310) & (020n-402) & . \\ \hline (1n-21000) & (011n-301) & (020n-402) & (020n-402) & (020n-310) & . \\ \hline .. & .. & .. & .. & .. & . \\ \hline \end{array}$$

The matrix elements are given in the notation eq. 61. From eq. 62 the full matrix $D^\eta(1,2)$ is constructed for any n : The numbers a, b are inserted from eq. 53 as functions of n . The diagonal elements indexed by $((i, i), i \geq 3)$ are repeated along the diagonal, the elements in the lines on top, and columns below the diagonal, are repeated in rows to the right and in columns downwards respectively by the same functions eq. 61 of n . Again $D^\eta(1,2)$ is orthogonal and symmetric, its square is the unit matrix. We find in general from eq. 53 for the entries of the first row and column of $D^\eta(1,2)$

$$(1n-21000) \rightarrow (1 + (n-2)a + b) = 0, \quad (63)$$

and so the $(n \times n)$ matrix $D^\eta(1,2)$ reduces to its $(n-1) \times (n-1)$ diagonal submatrix acting exclusively on the relative coordinates $(\eta_1, \eta_2, \dots, \eta_{n-1})$. In building orbital states from the symmetrized Gusev coordinates we must take care in the application of permutation operators.

References

- [1] Aguilera-Navarro V C, Kramer P, Moshinsky M
Harmonic oscillator states and the α -particle II. Configuration-space states of arbitrary symmetry. Ann of Physics (N Y) **54** (1969) 379—393
- [2] Avron J E, Herbst I W, and Simon B
Separation of center of mass in homogeneous magnetic fields Annals of Physics **114** (1978) 431–451
- [3] Bargmann V and Moshinsky M
Group theory of harmonic oscillators (I).
Nuclear Physics **18** (1960) 697–712
- [4] Bargmann V and Moshinsky M
Group theory of harmonic oscillators (II).
Nuclear Physics **23** (1961) 177–199
- [5] Barut A O and Raczka R
Theory of group representations and applications.
PWN Polish Scientific Publishers, Warsaw (1977)
- [6] Edmonds A R
Angular momentum in quantum mechanics.
Princeton University Press. Princeton (1957)
- [7] Escobar-Ruiz M A and Turbiner A V
Two charges on plane in a magnetic field I. Quasi-equal charges and neutral quantum system at rest cases.
Ann Phys **340** (2014) 37–59
- [8] Grossmann F and Kramer T
Spectra of harmonium in a magnetic field using an initial value representation of the semiclassical propagator.
J Phys A **44** (2011) 445309
- [9] Gusev A et al.
Symbolic-numerical algorithm for generating cluster eigenfunctions: identical particles with pair oscillator interactions. In: Computer Algebra in Scientific Computing, Springer, Berlin (2013) 155–168
- [10] Hamermesh M
Group theory and its application to physical problems.
Addison-Wesley, Reading (1962) 182–278

- [11] Johnson B R, Hirschfelder J O, and Yang K-H
Interaction of atoms, molecules, and ions with constant electric and magnetic fields. Rev Mod Phys **55** (1983) 109–153
- [12] Klama S and Mishchenko E
Two electrons in a quantum dot: a semiclassical approach.
 J. Phys.: Condens. Matter **10** (1998) 3411–3416
- [13] Kohn W
Cyclotron Resonance and de Haas-van Alphen Oscillations of an Interacting Electron Gas.
 Phys Rev **123** (1961) 1242–1244
- [14] Kramer P and Moshinsky M
Group theory of harmonic oscillators (III): States with permutational symmetry.
 Nuclear Physics **82** (1966) 241–273
- [15] Kramer P, John G and Schenzle D
Group theory and the interaction of composite nucleon systems.
 Vieweg, Braunschweig (1971)
- [16] Kramer P and Moshinsky M
Group theory of harmonic oscillators (IV): Dynamics of the 2,3, and 4 particle systems. Nuclear Physics **A 107** (1968) 481–522
- [17] Kramer P and Moshinsky M
Group theory of harmonic oscillators and nuclear structure. in: Group theory and its application,
 Ed E M Loebl, Academic Press, New York (1968) 340–368
- [18] Kramer P
Permutation group in light nuclei. In: Symmetry properties of nuclei, Proc 15th Solvay Conf. on Physics 1970, Gordon and Breach, New York (1974) 211–232
- [19] Kramer P, Kramer T, and Man’ko V I
Propagation in time of some classical/quantum systems and Nielsen’s conserved quantity.
 Phys Scr **79** (2009) 055006
- [20] Kramer T
Two interacting electrons in a magnetic field: comparison of semiclassical, quantum, and variational solutions.
 AIP Conference Proceedings **1323** (2010) 178

- [21] Kramer T, Krueckl V, Heller E J and Parrott R E,
Self-consistent calculation of electric potentials in Hall devices.
Phys Rev B **81** (2010) 205306
- [22] Kramer T, Kreisbeck C, Krueckl V, Heller E J, Parrott R E and Liang C-T
Theory of the quantum Hall effect in finite graphene devices.
Phys Rev B **81** (2010) 081410(R)
- [23] Kramer T
Interacting electrons in a magnetic field: mapping quantum mechanics to a classical ersatz-system.
AIP Conference Proceedings **1488** (2012) 394
- [24] Laughlin R
Anomalous quantum Hall effect: an incompressible quantum fluid with fractionally charged excitations.
Phys Rev Lett **50** (1983) 1395–1398
- [25] Moshinsky M and Quesne C
Oscillator systems. in: Symmetry properties of nuclei, Proc 15th Solvay Conf. on Physics 1970. Gordon and Breach, New York (1974) 233–300
- [26] Moshinsky M and Smirnov Y
The harmonic oscillator in modern physics.
Harwood Academic Publishers, Amsterdam (1996)
- [27] Muhandiramge R and Wang J
Electronic Structure of Multi-Electron Quantum Dots.
Mathematica journal **10:2** (2006) 396–414
- [28] Muhandiramge R D and Wang J
Spinadapted states: A basis for quantum dot structure calculation. International journal of quantum chemistry **106.1** (2006) 27–53
- [29] Su B, Goldman V J, and Cunningham J E
Evidence for spin singlet-triplet transitions of two electrons in a quantum dot observed via single-electron tunneling Surf Sci **305** (1994) 566–570
- [30] Taut M
Two electrons in a homogeneous magnetic field: particular analytical solutions.
J Phys A: Math Gen **27** (1994) 4723–4724
- [31] Tavernier M B et al.
Four-electron quantum dot in a magnetic field.
Phys. Rev B **68** (2003) 205305

- [32] Simonović N S
Three Electrons in a Two-Dimensional Parabolic Trap: The Relative Motion Solution.
 Few-Body Systems **38** (2006) 139–145
- [33] Verçin A
Two anyons in a static, uniform magnetic field. Exact solution.
 Physics Letters B **260** (1991), 120–124
- [34] Wagner M, Merkt U, and Chaplik A V
Spin-singlet spin-triplet oscillations in quantum dots.
 Phys Rev B **45** (1992) 1951–1954
- [35] Weyl H
The theory of groups and quantum mechanics. Dover, New York (1930)
- [36] Wigner E P
Group theory and its application to the quantum mechanics of atomic spectra.
 Academic Press, New York (1959)
- [37] Yannouleas C and Landman U
Quantal molecular description and universal aspects of the spectra of bosons and fermions in the lowest Landau level.
 Phys. Rev. A **81** (2010) 023609
- [38] Yukich J N, Kramer T, and Bracher C
Observed photodetachment in parallel electric and magnetic fields.
 Phys. Rev. A **68** (2003) 033412